

Industrial Technologies Program

Advances in Process Intensification through Multifunctional Reactor Engineering

Novel Reactor Concept Promises Increased Efficiency

Process intensification is a key strategy that the chemical industry is adopting for increasing energy efficiency and profitability. Multifunctional reactors (i.e., chemical reactors that integrate other functions such as separations) form the cornerstone of process intensification. Catalytic distillation is the classic example of multifunctional reaction engineering. However, no multiphase catalytic reactors currently operate in the novel mode that is the subject of this project, and no three-phase (vapor/liquid/liquid) commercial reactors exist for this mode. Existing systems are oversized and operate at less than optimal efficiency.

The novel multiphase catalytic reactor designs that result from this project will offer the chemical industry significant improvement in energy efficiency and process performance through enhanced mass and heat transfer. The technology will allow for optimization of existing trickle-bed reactors, such as refinery hydrotreaters. Other processes that could benefit include those that utilize liquid catalysts such as phosphoric acid, nitric acid, or ionic liquids. Applications that could benefit include 1) higher capacity vapor/liquid catalytic downflow reactors with fixed-bed

catalyst systems, 2) vapor/liquid/liquid reactors in which the catalyst is one of the liquid phases or is contained in one of the liquid phases, and 3) vapor/liquid upflow reactors utilizing a homogeneous catalyst slurry.

Multifunctional Reactor



Over the last decade, Sandia's Slurry Bubble-Column Reactor (SBCR) testbed has been successfully used to support indirect liquefaction studies.

Sandia's Slurry Bubble-Column Reactor (SBCR) testbed

Benefits

- *Potential energy savings of 83 trillion Btu per year by 2020*
- *Fuel and electricity savings of at least 50%*
- *Improved reactor performance through more efficient mass and heat transfer*
- *Significantly reduced solid wastes through reduction in acid used for alkylation*

Applications

The process is being developed specifically for acid catalyzed C4 paraffin/olefin alkylation. However, these novel multiphase catalytic reactors could be used in other processes across the chemical industry. In particular, processes that use liquid catalysts such as phosphoric acid, nitric acid, or ionic liquids will enjoy significant improvements in performance and efficiency.

Project Partners

- *Chemical Research and Licensing Company
Pasadena, TX*
- *ABB Lummus*
- *Sandia National Laboratories
Albuquerque, NM*

Industrial Technologies Program

Project Description

Goal: The overall objective of the project is to develop the knowledge and tools required to develop and scale a novel multiphase, catalytic reactor for acid catalyzed C4 paraffin/olefin alkylation to industrial dimensions.

The focus of the project will be on the sulfuric-acid-catalyzed C4 paraffin/olefin alkylation reaction, which is a key process area in which to obtain energy savings via efficient mixing of fluids. An efficient system would obtain high mass transfer between the process liquids by utilizing a novel flow regime as opposed to impeller mixing devices.

Experiments have demonstrated that the proposed mode of operation in vessels containing structured packing material can enhance inter-phase mass transfer. Important physical phenomena occurring in this environment include evaporation, condensation, mass transfer between the phases, chemical reactions, heat release and transfer, and three-phase flow through a structured material. Normally in this process, the interaction between the hydrocarbon liquid and the acid phase limits reaction rate, while the absence of effective fluid/fluid contact leads to the formation of undesired heavier molecular weight. The novel mode of operation overcomes these negative effects with less energy expenditure than the traditional approach of using high-shear mixers.

Activities:

This project will consist of interrelated experimentation (bench-scale and pilot-scale) and modeling tasks. The bench-scale experiments will focus on materials characterization, process chemistry, and structure-scale hydrodynamics. The pilot-scale experiments will focus on vessel-scale hydrodynamics. Project partners will also investigate the transition between trickle-flow and other modes and the characteristics of the changes. They will develop detailed models of structure-scale processes, which they will incorporate into a vessel-scale hydrodynamics model.

Milestones

Year 1:

- 1) Simulant system for pilot-scale experiment
- 2) Bench-scale hydrodynamics experiment
- 3) Pilot-scale pulse-flow hydrodynamics experiment

Year 2:

- 1) Validated model of bench-scale hydrodynamics
- 2) Initial data sets from pilot-scale experiments

Year 3:

- 1) Model of pilot-scale hydrodynamics
- 2) Comprehensive pilot-scale data set showing benefits
- 3) Validation of scaling approach
- 4) Final report documenting validated scale-up approach
- 5) Transition to commercial-scale design

For Additional Information, please contact:

Dr. Arvids Judzis
Vice President, Commercial
Development
Chemical Research and Licensing
Phone: (281) 474-0671
E-mail: AJudzis@cd-tech.com

For Program Information, please contact:

Brian Valentine
Industrial Technologies Program
U.S. Department of Energy
1000 Independence Ave., SW
Washington, D.C. 20585
Phone: (202) 586-7543
Fax: (202) 586-1658
E-mail: brian.valentine@ee.doe.gov

Please send any comments, questions, or suggestions to webmaster.eren@nrel.gov

Visit our home page at www.eere.energy.gov/industry

**Industrial Technologies Program
Energy Efficiency and Renewable Energy
U.S. Department of Energy
Washington, D.C. 20585**



U.S. Department of Energy
Energy Efficiency
and Renewable Energy

March 2004